1,5-Dimethyl-6-phenyl-1,6-dihydro-3-pyridinecarbonitrile

	2/531-49-3 DTXSID3029/54/				
Model Performance					
Model		Data			

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 1.20e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.98e-01

Confidence level: 3.73e-01

Nearest Neighbors from the Training Set

Image not found

Isouron

Measured: 1.20e-06 Predicted: 1.37e-06 Image not found

DEET

Measured: 2.07e-04 Predicted: 1.22e-03

Image not found

Diphenyl oxide

Measured: 7.39e-04 Predicted: 7.14e-03